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Studies on Thickness and Internal Quantum Efficiency of $Cs_2AgBiBr_6$ Based Double Perovskite Material for Photovoltaic Application

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The lead-free double perovskites have recently emerged as promising alternative material for solar cell application. It exhibits encouraging optoelectronic properties, high environmental stability and low toxicity. The double perovskite having two different cations are non-toxic alternatives. The double perovskite $Cs_2AgBiBr_6$ has good optical and electronic features. Therefore, it has been used for high-efficiency optoelectronic devices. In this manuscript, we report optimization of active layer thickness of double perovskite $Cs_2AgBiBr_6$ for photovoltaic application. For the study, a device FTO/TiO_2/$Cs_2AgBiBr_6$/Spiro-OMeTAD/Cu was designed. The Solar Cell Capacitance Simulator (SCAPS-1D) was used for one dimensional simulation and analysis. The active layer of 0.1 to 1 μm was used for the study and PCE, V_{oc}, J_{sc} and FF were obtained using simulation. The optimum active layer thickness was found to be between 0.20 μm to 0.4 μm. The maximum PCE of 3.78 % was found. The solar cell performance can be improvised further by optimizing the defect density of the active layer. Also, the effects of ETL and HTL layer thickness can be further observed for enhancement of PCE. Overall, the encouraging simulation results achieved in this study will provide insightful guidance in replacing commonly used cancerous Pb-based perovskite with eco-friendly, highly efficient inorganic perovskite solar cell.

Keywords: SCAPS-1D, Double perovskite, Solar cell, Photovoltaic, Optimization, Electron transport layer.

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1. INTRODUCTION

The lead (Pb) based hybrid perovskite materials have been used extensively for solar cells because of high power conversion efficiency of around 25 %. The toxic property of lead (Pb) creates a hurdle in fabricating the cells. Generally, a perovskite solar cell architecture consists of an electron transport layer (ETL) and a hole transport layer (HTL) which in turn maximizes power conversion efficiency (PCE) [1]. The volatility of the organic cation is considered to be a significant contributor to instability, which should be improved using inorganic cations [2]. For these reasons, the search for alternative inorganic perovskites employing fewer toxic metals is of paramount importance [3-5]. In this landscape, double perovskites have recently emerged as particular promising alternatives exhibiting encouraging optoelectronic properties, high environmental stability, and low toxicity. In particular, the double perovskite $Cs_2AgBiBr_6$ has been the subject of much fundamental material characterization and initial application in photodetectors and photovoltaic devices [6-11]. In this present work, we have studied the solar cell device with Cesium based inorganic absorbing material $Cs_2AgBiBr_6$ for the best photovoltaic performance under the optimum absorbing layer thickness. The titanium dioxide (TiO_2) has been used as ETL and Spiro-OMeTAD as HTL materials.

2. METHODOLOGY

2.1 Ziggurat of the Devices

The ziggurat of the PSC is shown in Fig. 1a. TiO_2 has been used as ETL and double perovskite ($Cs_2AgBiBr_6$) material is used as active layer. The Spiro-OMeTAD is used as HTL. The PSC has two interfacial layers. The energy level of the device is shown in Fig. 1b.

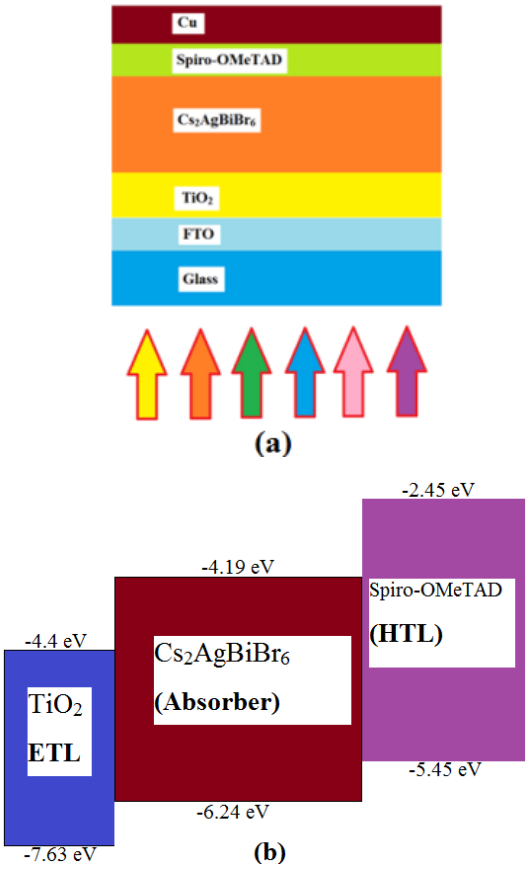

Fig. 1 – Device architecture (a), band alignment (b)

2.2 Simulated Parameters

SCAPS-1D is a one-dimensional solar cell capaci-

The results were presented at the International Conference on Innovative Research in Renewable Energy Technologies (IRRET-2021)

tance simulator developed at University of Gent, Belgium [12]. The material parameters used in this simulation are listed in Table 1. The values were chosen from literature and the previous simulation works [13-17]. Electron and hole thermal velocities are kept constant at 10^7 cm·s^{-1} [18]. Neutral type and donor type defects are considered for HTL and absorber layer, respectively. But for both ETL and window layer, acceptor type defects are considered. Absorber layer and ETL have variable total defect density (N_t), whereas HTL has fixed N_t. All interfacial layers have neutral type defects and variable trap densities [18].

Table 1 – SCAPS-1D input material parameters used in the solar cell simulation [8-11]

Parameters	Window layer FTO	ETL TiO_2	Absorber layer $Cs_2AgBiBr_6$	HTL Spiro-OMeTAD
Thickness, μm	0.2	0.3	0.1-1	0.3
Bandgap (E_g), eV	3.2	3.23	2.05	3.0
Electron affinity (χ), eV	4.4	4.26	4.19	2.45
Relative permittivity (ε_r)	9.0	9.0	5.80	3.0
CB effective density of states (N_c), cm^{-3}	$2.2{\cdot}10^{18}$	$2.0{\cdot}10^{18}$	$1.0{\cdot}10^{16}$	$2.2{\cdot}10^{19}$
VB effective density of states (N_v), cm^{-3}	$1.8{\cdot}10^{19}$	$1.8{\cdot}10^{20}$	$1.0{\cdot}10^{16}$	$1.8{\cdot}10^{19}$
Electron mobility (μ_n), cm^2·V^{-1}· s^{-1}	20	4	11.81	$2.0{\cdot}10^{-4}$
Hole mobility (μ_p), cm^2·V^{-1}·s^{-1}	10	2	0.49	$2.0{\cdot}10^{-4}$
Donor density (N_d), cm^{-3}	$1.0{\cdot}10^{18}$	$6.0{\cdot}10^{19}$	$1.0{\cdot}10^{19}$	0
Acceptor density (N_a), cm^{-3}	0	0	$1.0{\cdot}10^{19}$	$1.0{\cdot}10^{18}$
Defect density (N_t), cm^{-3}	$1.0{\cdot}10^{15}$	$1.0{\cdot}10^{18}$	$9.1{\cdot}10^{16}$	$1.0{\cdot}10^{14}$

3. RESULTS AND DISCUSSION

3.1 Effect of the Thickness of Active Material Layer

The thickness of the active material layer is a crucial parameter to regulate the efficiency of a solar cell. In order to find out the optimum thickness of the active layer, it is varied from 0.1 μm to 1 μm while keeping the other material parameters constant. The QE, FF, V_{oc}, and J_{sc} are simulated against varying active layer thickness (Fig. 2). From the *J-V* characteristics, the J_{sc} and V_{oc} can be found out directly. The active layer thickness studied for simulation is varied from 0.1 to 1 μm with 0.1 μm step. It has been found out that the thickness of the double perovskite active material should be less than the electron diffusion length [19].

It causes the electron and holes to reach the respective electrodes to generate the power. Thus, increasing the layer thickness causes more light absorption and as a result higher J_{sc}, V_{oc}, PCE, maximum power generation can be obtained [20]. As a result, some of the photo-generated electron-hole pairs recombine at the back contact, leading to decrement in the back contact recombination current density with every increment of thickness of the absorbing layer. It is evident from Fig. 2a and Fig. 2b that the parameters J_{sc} and PCE increases with the increase in the thickness of the Double Perovskite absorber layer ($Cs_2AgBiBr_6$) initially and reaches its peak value between 0.2 μm and 0.4 μm. But further increase in the thickness of the absorber layer, it could be seen that the values of J_{sc} and PCE do not increase.

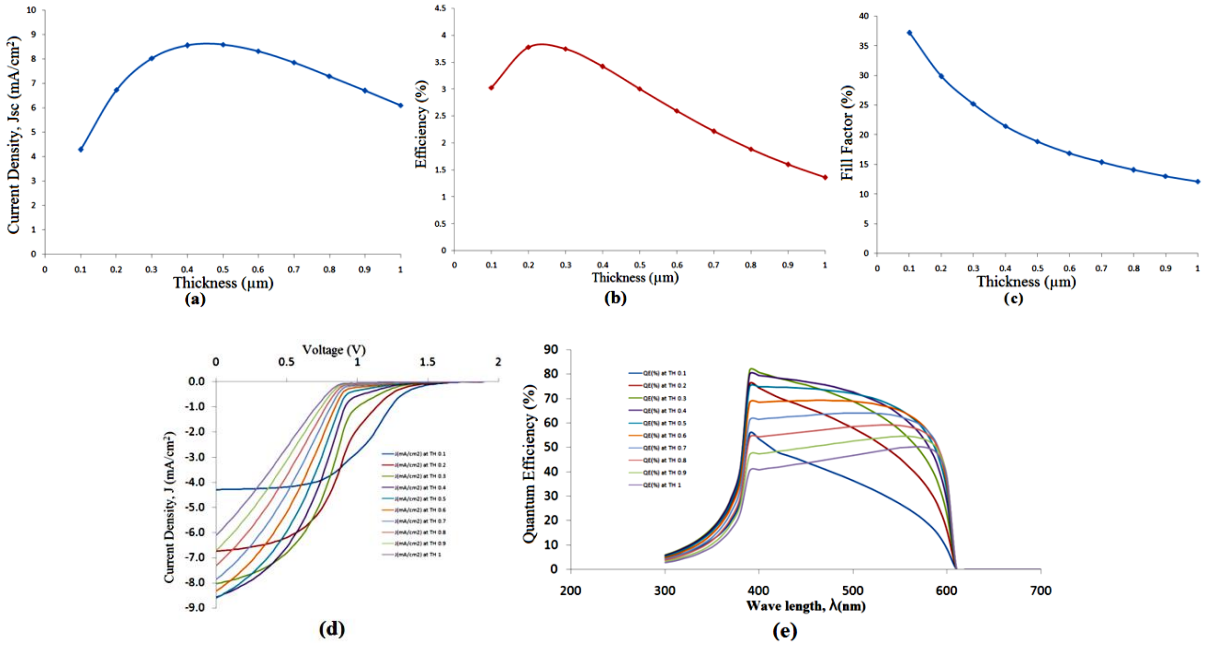

Fig. 2 – J_{sc} vs thickness (a), η vs thickness (b), FF vs thickness (c), *V-J* characteristics (d), QE vs λ (e)

This may be due to increase in the carrier diffusion lengths. Also, the generated electron and hole pair cannot reach to the space charge region during their life span and leads to bulk recombination of carriers [21, 22]. A thicker layer can absorb more photon as a result higher conversion efficiency is expected with an active layer optimized between 0.2 and 0.4 μm for better performance of the solar cell and for higher PCE [23]. The PCE has reached a maximum value of 3.78 %. The values of the maximum PCE dependent parameters are J_{sc} = 6.737103 mA/cm^2, FF = 29.88 %, V_{oc} = 1.8782 V. The efficiency followed the shape of a bell curve with increasing absorber layer thickness. The absorber layer thickness with maximum PCE is found to be 0.2 μm. In Fig. 2d we present the *J-V* curves for each film thickness. In Fig. 2e, the spectral response generation with different wavelength of the double perovskite absorbing layer is shown. The efficiency of a solar cell is generally quantified by internal quantum efficiency (IQE) and external quantum efficiency (EQE, also known as classical efficiency). The EQE takes optical performance of the solar cell along with the ration of charge generation with respect to incident light photons. On the other hand, the IQE is the ratio of electrons collected as photo current to the number of absorbed photons of a particular wavelength. IQE will help predict the total current generation under solar spectrum as well as the range of solar spectrum utilized for power generation by the active material [23, 24]. On the other hand, the classical efficiency or EQE may be studied in future for detailed analysis. The effect of light illumination wavelength (from 200 to 700 nm light wavelength) on the perovskite active layer performance was studied. IQE is the part of wavelength which is converted into the electron-hole pair and collected as charge carrier from the active material [25]. The double perovskite active layer gives maximum quantum efficiency of 81.5 % for 0.3 μm thickness of active layer, as shown in Fig. 2e. The best spectral response was obtained from 380 nm to 600 nm.

4. CONCLUSIONS

In this research work, lead-free double perovskite ($Cs_2AgBiBr_6$) as the absorber layer is investigated through SCAPS-1D simulation.

The configuration of the PSC is glass substrate/FTO/TiO_2/$Cs_2AgBiBr_6$/Spiro-OMeTAD/Cu. The effect of absorber layer thickness on the PSC performance is discussed. The simulation results reveal that the active material performance depends upon the thickness. The optimal absorber layer thickness was found to be 0.2 μm for the double perovskite $Cs_2AgBiBr_6$ material. The best spectral response for the double perovskite material was found to be at 390 nm. This concludes that, the material is active in visible region of the solar spectrum.

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Дослідження товщини та внутрішньої квантової ефективності подвійного перовскітного матеріалу на основі $Cs_2AgBiBr_6$ для фотоелектричних додатків

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Безсвинцеві подвійні перовскіти нещодавно стали перспективним альтернативним матеріалом для застосування в сонячних елементах. Вони мають обнадійливі оптоелектронні властивості, високу екологічну стабільність та низьку токсичність. Подвійний перовскіт, що має два різні катіони, є нетоксичною альтернативою. Подвійний перовскіт $Cs_2AgBiBr_6$ має гарні оптичні та електронні характеристики. Тому його застосовували для високоефективних оптоелектронних пристроїв. У статті мова йде про оптимізацію товщини активного шару подвійного перовскіту $Cs_2AgBiBr_6$ для фотоелектричних додатків. Для дослідження було розроблено пристрій FTO/TiO_2/$Cs_2AgBiBr_6$/Spiro-OMeTAD/Cu. Симулятор ємності сонячних елементів (SCAPS-1D) використовували для одновимірного моделювання та аналізу. Для дослідження використовували активний шар товщиною 0,1-1 мкм, а значення PCE, V_{oc}, J_{sc} та FF отримували за допомогою моделювання. Оптимальна товщина активного шару становить від 0,2 до 0,4 мкм. Максимальне значення PCE виявилося рівним 3,78 %. Ефективність сонячних елементів може бути покращена додатково шляхом оптимізації щільності дефектів активного шару. В подальшому також можна спостерігати ефекти товщини шарів ETL та HTL для покращення PCE. Загалом, обнадійливі результати моделювання, отримані в дослідженні, нададуть корисні рекомендації щодо заміни часто використовуваного шкідливого перовскіта на основі свинцю екологічно чистим, високоефективним неорганічним перовскітним сонячним елементом.

Ключові слова: SCAPS-1D, Подвійний перовскіт, Сонячний елемент, Фотоелектричний, Оптимізація, Електронний транспортний шар.